O,O-Diethyl dithiophosphate

298-06-6 | DTXSID6027133

Model Performance

Model		Data	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.44e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.29e-01

Confidence level: 4.91e-01

Nearest Neighbors from the Training Set

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.alpha.-
[(Cyanomethoxy)imino]benzeneacetonitrile
Measured: 5.13e-04
Predicted: 5.60e-02

Image not found

Benzyl acetate
Measured: 2.06e-02
Predicted: 1.22e-01

Image not found

alpha-Methoxyacetophenone
Measured: 1.73e-01
Predicted: 1.23e-01

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Ethyl benzoate
Measured: 4.79e-03
Predicted: 9.44e-02